

Sodium 3-nitrobenzenesulfonate
127-68-4 | DTXSID2027048

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.42 mol/L

Global applicability domain: Inside

Local applicability domain index: 3.66e-01

Confidence level: 6.11e-01

Nearest Neighbors from the Training Set

Image not found

2-Methyl-5-nitrobenzenesulfonic acid

Measured: 3.07

Predicted: 2.77

Image not found

2-Hydroxyethanesulfonic acid

Measured: 7.93

Predicted: 6.22

Image not found

4-Methylbenzenesulfonic acid

Measured: 3.60

Predicted: 2.37

Image not found

4-Aminobenzenesulfonic acid

Measured: 6.24e-02

Predicted: 1.78e-01